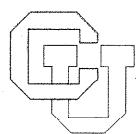


Meta-domains for Automated Model Building *

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CU-CS-898-99



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Meta-domains for Automated Model Building

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Abstract

We present a new knowledge representation and reasoning framework for modeling nonlinear dynamical systems. The goals of this framework are to smoothly incorporate varying levels of domain knowledge and to tailor the search space and the reasoning methods accordingly. In particular, we introduce a new structure for automated model building known as a *meta-domain* which, when instantiated with components, tailors the space of candidate models to the system at hand. The *xmission-line* meta-domain, for instance, generalizes the notion of an electrical transmission line, using an iterative template to build models; it may be customized into specific model-building domains ranging from mechanical vibrations to thermal conduction. We combine this with ideas from generalized physical networks, a meta-level representation of idealized two-terminal elements, and a hierarchy of qualitative and quantitative analysis tools, to produce dynamic modeling domains whose complexity naturally adapt to the amount of available information about the target system.

Introduction

System identification (SID) is the process of identifying a dynamic model of an unknown system. The challenges involved in automating this process are significant, as applications in different fields of science and engineering demand different kinds of models and modeling techniques. System identification entails two steps: *structural identification*, wherein one ascertains the general form of the model as described by an ordinary differential equation or ODE (e.g., $a_1\ddot{\theta} + a_2 \sin \theta = 0$ for a simple pendulum), and then *parameter estimation*, in which one finds specific parameter values for the unknown coefficients that fit that model to observed data (e.g. $a_1 = 1.0$, $a_2 = -98.0$). For nonlinear systems, parameter estimation is difficult and structural identification is even harder; AI techniques can be used to automate the former(Bradley, O'Gallagher, & Rogers 1998),

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but the latter has, until now, remained the purview of human experts.

A central problem in any automated modeling task is that model complexity, and hence the size of the search space, is exponential in the number of model components unless severe restrictions are placed on the model-building process. A good compromise between *black-box* modeling, which uses no domain knowledge but has a prohibitively large search space, and *clear-box* modeling, where the modeler knows a great deal about the system, is *gray-box* modeling. Here, partial information about the internals of the box—e.g., whether the system is electronic or viscoelastic—is used to prune the search space to a reasonable size. The key to making gray-box modeling of nonlinear dynamical systems practical is a flexible knowledge representation scheme that adapts to the problem at hand. Domain-dependent knowledge can drastically reduce the search-space size but its applicability is limited.

Our solution combines a representation that allows for different levels of domain knowledge, a set of reasoning techniques that are appropriate to each level, and a control strategy that invokes the right technique at the right time. In particular, we introduce a new structure for automated model building known as a *meta-domain* which, when instantiated with domain components, tailors the model generation search space to an identification task. To increase a meta-domain's applicability and utility, we also incorporate ideas from *generalized physical networks*(Sanford 1965), a meta-level representation of idealized two-terminal elements, traditional compositional model building(Falkenhainer & Forbus 1991), and qualitative reasoning(Weld & de Kleer 1990). The intent is to span the spectrum between highly specific frameworks that work well in a single, limited domain (e.g., a spring/dashpot vocabulary for modeling simple mechanical systems) and abstract frameworks that rely heavily upon general mathematical formalisms at the expense of having large search spaces.

Meta-domains for Model Building

Theoretically, an automated system identification tool could rely solely upon a brute-force model generator for its structural identification phase and a nonlinear pa-

rameter estimator for its testing phase. However, many implementation issues make this idea wholly impractical. Parameter estimation is extremely expensive and even simple application domains have an exponential number of valid models. Consider, for example, all of the permutations of connecting a single electrical resistor, capacitor, and inductor together in parallel and/or series. Although the complete set of permutations does describe all possible models that can be built with this set of components, the number of functionally different models in the set is significantly less. The keys to the structural identification phase are (1) to create an appropriate set of models that describes interesting behaviors without creating an overly large search space and (2) to test them using abstract, high-level reasoning whenever possible.

Unfortunately, the knowledge required to accomplish this is quite heterogeneous, varying greatly in utility, applicability, and form. More-restrictive domains tend to admit more-powerful analysis tools and have much smaller search spaces. In linear mechanical systems, an impulse response shows the natural resonant and anti-resonant frequencies as spikes, and the *mode shapes* between those spikes show whether a vibrating mechanical system is mass- or stiffness-dominated (Juang 1994). In viscoelastics, an even more restrictive domain, three qualitative properties of a “strain test” reduce the search space of models to linear (Capelo, Ironi, & Tentoni 1998). Assessing how and when to apply these types of tools and domain knowledge is a non-trivial knowledge representation and reasoning problem.

Our term for the specific knowledge and tools used to automatically generate and test models is a *model-building domain*, which contains:

- A set of prototypical domain components
- A model generator—a function that combines components into candidate models
- A set of data analysis tools that create qualitative and quantitative knowledge appropriate to the system at hand
- A set of rules and associated reasoning modes that apply this knowledge to discover inconsistencies between the candidate model and the unknown system.

Model building domains are similar in that they begin with a set of components and return a candidate ODE model; they differ not only in their generality (and thus the size of their search spaces) but also in the type and utility of their analysis tools, reasoning modes and rules.

Creating individual model-building domains from scratch for each specific application is inefficient as much of the model generation knowledge and many of the tools actually apply to more than one domain. Organizing model-building domains into a hierarchy of generality allows more-general domains, such as *linear-systems*, to be easily customizable into more-specific ones, such as *linear-mechanical-systems*. Analysis tools may also exploit this hierarchy. Non-linear time-series analysis, for example, can reveal the

lower bound on the dimensionality of any system of ODEs, whereas a step response test is only useful in modeling linear systems, and a creep test is even more domain-specific. Model-building components may take advantage of this hierarchy as well by using generalized physical networks (GPNs), an energy based modeling paradigm similar to bond graphs. Here, similarities between components and properties in different domains are brought out through generalized components such as *linear-resistance*, which models energy dissipation. This abstract component may be customized—into *linear-resistor*, *linear-damper*, etc.—depending upon the application. Available domain knowledge expands or contracts based upon the problem, selectively sharpening the model in *appropriate and useful* ways.

Hierarchical knowledge also exists for the model generation phase, which is critical, as haphazardly connecting arbitrary components creates an exponential number of candidate models. One way of reducing this number is to use a *meta-domain*: a general framework that arranges components into models by relying on modeling techniques that transcend individual application domains. This paper introduces two such meta-domains: *linear-plus* and *xmission-line*. The *linear-plus* meta-domain takes advantage of fundamental linear-systems properties that allow the linear and nonlinear components to be treated separately under certain circumstances, which dramatically reduces the model search space. The *xmission-line* meta-domain generalizes the notion of building models using an iterative pattern, similar to a standard model of a transmission line, which is useful in modeling distributed systems. Meta-domains can be customized into more-specific domains or used directly; we demonstrate both approaches in the following section. We chose this pair of meta-domains as a good initial set because they cover a wide variety of practical engineering problems. We are exploring other possible meta-domains, especially for the purposes of modeling nonlinear networks.

Applying Meta-domains in PRET

PRET (Bradley & Stolle 1996) is an automatic SID tool that constructs ordinary differential equation (ODE) models of lumped-parameter continuous-time nonlinear dynamic systems. It takes a generate-and-test approach, using a small, powerful domain theory to build models, and then uses a body of mathematical and physical knowledge encoded in first-order logic to test those candidate ODEs against behavioral observations of the target system. Unlike other AI modeling tools—most of which use libraries to build models of small, well-posed problems in limited domains—PRET builds models of nonlinear systems in multiple domains and uses sensors and actuators to interact directly and automatically with the target system. PRET relies heavily on the notions of model-building domains and meta-domains. It currently incorporates five specific GPN-based modeling domains:

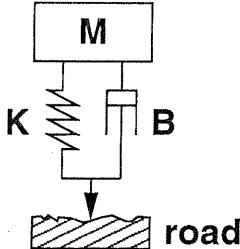


Figure 1: A one-degree-of-freedom quarter-vehicle model that includes a shock absorber—a viscous damping element, B—connected in parallel with a spring, K, and the loading effects of the car, M.

mechanics, viscoelastics, linear-electronic, linear-rotational, and linear-mechanical. These domains are dynamic: if a domain does not contain a successful model, it automatically expands to include additional components. For example if PRET fails to find a model in the linear-electronics domain, whose basic components include {linear-resistor, linear-capacitor}, that domain automatically expands to include linear-inductor. If a user wants to apply PRET to a system that does not fall in an existing domain, he or she can either build one from scratch—a matter of making a list of components and connectors—or use one of the meta-domains. PRET's two meta-domains, linear-plus and xmission-line, exploit modeling techniques that transcend individual application domains: linear system fundamentals in the former and an iterative structure in the second. PRET has successfully been applied to a variety of system identification tasks, ranging from textbook engineering problems to a radio-controlled car used in a deployed robotics system(Bradley, O'Gallagher, & Rogers 1998). This section presents two examples that demonstrate how domains and meta-domains contribute to this process.

Modeling a Shock Absorber

Hydraulic shock absorbers, common in modern commercial vehicles, are complex nonlinear devices whose behavior depends upon the amplitude and frequency of the imposed motion. Accurate mathematical models of this behavior are key to realistic vehicle simulations and active-suspension controllers. Shock-absorber models normally come in two forms: either as a stand-alone shock absorber—typically just a connected spring and damper element—or as part of a quarter-vehicle model, where the loading effects of one quarter of the vehicle are included. The effects of different shock absorbers in one- and two-degree-of-freedom quarter vehicle models may be found in (Langlois & Anderson 1997); the behavior of five damper model variants, such as “no spring,” “velocity-dependent damping,” or “no linear spring,” is described by (Besinger, Cebon, & Cole 1997). This is exactly the kind of expert reasoning that motivated the design of the domain knowledge framework described here; these kinds of similarities make it easy for engi-

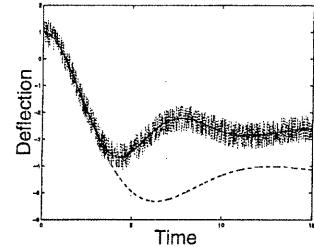


Figure 2: Step responses of (a) a hydraulic shock absorber (dotted) (b) an unsuccessful candidate model with a linear spring (dashed) and (c) a successful model, which incorporates a cubic spring (solid).

```
(find-model
  (domain linear-mechanics) ...
  (hypotheses
    (<force> (* k (cube (integral <v>))))
    (<force> (* b <v>)))
  (drive (<force> d))
  (observations
    (numeric (<time> <position>)
      ((0 1.3) (0.1 1.2) ...))) ...)
```

Figure 3: A find-model call for the shock absorber. The state variable $\langle v \rangle$ is velocity (i.e. $v = \frac{dx}{dt}$, where $x = \langle \text{position} \rangle$ is the deflection from equilibrium). The numeric observation is the noisy dotted time series shown in the previous figure.

neers to use PRET on real problems.

As shown in the find-model call fragment in Figure 3, the user initializes PRET on this modeling problem by specifying the domain (linear-mechanics), a few hypotheses (a spring force that obeys a cubic version of Hooke's law and a viscous friction term), a constant drive term that represents a constant normal force on the suspension, and a noisy time-series measurement of the deflection (shown graphically in Figure 2(a)). By default, the linear-mechanics domain includes linear damping, inertia, and spring components, so the user need not enter them explicitly; PRET's model generator will automatically include them along with the user-specified hypotheses. Geometric pre-processing of the numerical observation shows that the state variable $\langle x \rangle$ undergoes a damped oscillation to a fixed point. From these facts, PRET's model tester(Stolle & Bradley 1998) deduces (among other things) that the order of any linear model must be at least two. This qualitative information lets PRET immediately rule out the first dozen or so candidate models. Proceeding to slightly more complex ODEs, PRET generates the model $a\ddot{x} + b\dot{x} + cx + d = 0$, which is made up of three built-in domain hypotheses and the user's drive hypothesis. Its model tester cannot rule out this model using qualitative reasoning techniques, and so is forced to invoke its nonlinear parameter estimator to establish that the solution to this ODE, shown in Figure 2(b), does not match the numeric observation shown in Figure 2(a). After discarding a variety of other unsuccessful candidate models by various means, PRET eventually generates and tests the ODE $a\ddot{x} + b\dot{x} + cx + kx^3 + d = 0$. This model passes all qualitative and quantitative checks, and so is

returned as PRET's output:

```
... no refutation ...
(model ((= (+ (* (const a) (deriv (deriv <x>)))
              (* (const b) (deriv <x>))
              (* (const c) <x>)
              (* (const k) <x> <x> <x>)
              (const d)) 0)
        ((a 1.00) (b 0.50) (c 0.31) (k 0.024) (d 1.30))))
```

The **linear-mechanics** domain can be implemented in several ways. The easiest is to use the **linear-plus** meta-domain and add several domain-specific components: **linear-mass**, **linear-damping** and **linear-spring**. These are just the generalized components **linear-capacitance**, **linear-resistance** and **linear-inertia**—renamed in a manner that makes their meaning obvious to someone who would be using the **linear-mechanics** domain. Jargon matching is only a small part of the power of meta-domain customization, however; domain knowledge allows PRET to selectively sharpen its knowledge. If PRET knows that the system is linear and mechanical, for instance, the general component **linear-inertia** takes on the more-specific meaning associated with **linear-spring**, such as the knowledge that mechanical springs often have appreciable mass and internal friction that cannot be neglected.

Implementing the **linear-mechanics** domain using the **linear-plus** meta-domain has another very important advantage for problems like this, which have a few drive terms and a few nonlinear terms. **linear-plus** separates components into a linear and a non-linear set in order to take advantage of two fundamental properties of linear systems: (1) there are a polynomial number of unique *n*th-order linear ODEs(Brogan 1991), and (2) linear system inputs (drive terms) appear verbatim in the resulting ODE system. The first of these properties converts an otherwise-exponential search space to polynomial; functionally equivalent linear networks reduce to the same Laplace transform transfer function, which allows PRET to identify and rule out any ODEs that are equivalent to models that have already failed the test. The second property allows this meta-domain (and thus any specific domain constructed upon it) to handle a limited number of nonlinear terms by treating them as system inputs. As long as the number of nonlinear hypotheses remains small, the search space of possible models remains tractable.

One could also use the **linear-plus** domain directly for this problem simply by specifying a few extra hypotheses (e.g., $a\ddot{x}$, and so on). The only effect would be on PRET's run time, as it would no longer be able to use domain knowledge to streamline the generate and test phases. The best course of action is to use as much domain knowledge as possible, and PRET's layered domain/meta-domain framework is designed to make it easy to do so.

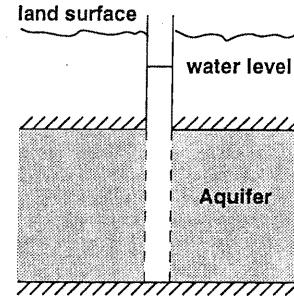


Figure 4: An idealized representation of an open well penetrating an artesian aquifer. The motion of the water level in the well is controlled by sinusoidal fluctuations of the pressure in the aquifer.

Water Resource Systems

Water resource systems are made up of streams, dams, reservoirs, wells, aquifers, etc. In order to design, build, and/or manage these systems, engineers must model the relationships between the inputs (e.g., rainfall), the state variables (e.g., reservoir levels), and the outputs (e.g., the flow to some farmer's irrigation ditch). To do this in a truly accurate fashion requires partial differential equations (PDEs) because the physics of fluids involves multiple independent variables—not just time—and an infinite number of state variables. PDEs are extremely hard to work with, however, so the state of the art in the water resource engineering field falls far short of that. Most existing water resource applications, such as river-dam or well-water management systems, use rule-based or statistical models. ODE models, which capture the dynamics more accurately than these simple models but are not as difficult to handle as PDEs, are a good compromise between these two extremes, and the water resource community has begun to take this approach(Bredehoeft, Cooper, & Papadopoulos 1966; Chin 2000). In this section, we use PRET to duplicate some of these research results and model the effects of sinusoidal pressure fluctuation in an aquifer on the level of water in a well that penetrates that aquifer. See Figure 4 for a schematic. This example is a particularly good demonstration of how domain knowledge and the structure inherited from the meta-domain let the model generator build systems without creating an overwhelming number of models. This is especially useful when none of PRET's existing domains matches a user's application area. This example also demonstrates how GPNs allow PRET to model a variety of systems using the same underlying representation and to incorporate the load effects easily and naturally into the model.

The first step in describing this modeling problem to PRET is to specify a domain. Because there is no built-in “water resource” domain, the user would have to choose (and perhaps customize) one of the meta-domains. For this problem, the choice is obvious, as the **xmission-line** meta-domain is specifically designed for this kind of *distributed* physics, which turns up in fluid flows, vibrating strings, gas acoustics, thermal conduc-

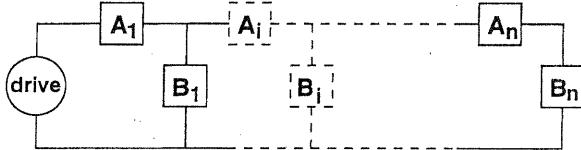


Figure 5: The *xmission-line* meta-domain allows PRET to use its lumped-element GPN components to model spatially distributed systems.

tion and diffusion, etc.(Ghausi & Kelly 1968). This meta-domain serves as a bridge between two very different paradigms. GPN components represent prototypical *lumped* elements, each of which models a single physical component, whereas a system like a transmission line or a guitar string can be thought of as an infinite number of small elements (the basis of a PDE model). Using the former to model the latter requires an incremental approach. In particular, one can approximate a spatiotemporally distributed system using an iterative structure with a large number of identical lumped sections, each of which corresponds to an ODE term. Figure 5 shows a diagram of this: a generalized iterative two-port network with n sections, each of which has a serial (A_i) and a parallel (B_i) component. In a basic model of an electrical transmission line, for example—whence the name of the *xmission-line* meta-domain—typical electrical parameters, such as resistance or inductance, are given in per-unit-length form, and the A_i and B_i would correspond to resistors and capacitors, respectively.

As in the shock absorber example, PRET's user can either customize the meta-domain or use it directly. For the well/aquifer problem, this customization would consist of renaming the general components *linear-capacitance*, *-inertia*, and *-resistance* to match the standard domain vocabulary; capacitive and resistive effects, in particular, simulate radial flow in an aquifer, and water mass is treated as inertia. (These concepts and equivalences, which appear in every textbook, are a routine part of a water-resource practitioner's knowledge.) The domain could be further customized based upon knowledge of the aquifer's forcing function; if the water's velocity changes slowly, for example, inertia effects can normally be ignored. For the purposes of demonstrating how one uses a meta-domain directly, however, we omit this customization in this example, so the *find-model* call of Figure 6 simply instantiates the *xmission-line* meta-domain.

This call differs from the previous examples in a variety of ways. This meta-domain has no built-in components; it only provides the template of an iterative network structure. PRET must therefore rely solely on user-specified hypotheses¹. State variables in hypotheses bear domain-independent names like *<effort>* and *<flow>*, rather than domain-specific ones like

¹In other domains, PRET uses power-series expansions if it runs out of user hypotheses. Since the basic paradigm in *xmission-line* is essentially a spatial expansion, a power-series expansion would be a duplication of effort.

```
(find-model
  (domain xmission-line)
  (state-variables (<well-flow> <flow>)) ...
  (hypotheses
    (<effort> (* c (integral <flow>)))
    (<effort> (* 1 (deriv <flow>)))
    (<effort> (* r <flow>)))
  (drive (<effort> (* da (sin (* df <time>))))))
  (observations
    (not-constant <well-flow>)
    (not-constant (deriv <well-flow>))
    (numeric (<time> <well-flow> (deriv <well-flow>))
      ((0 4.0 0.5) (0.1 4.25 0.6) ...)) ...)
```

Figure 6: A *find-model* call fragment for the well/aquifer example of Figure 4.

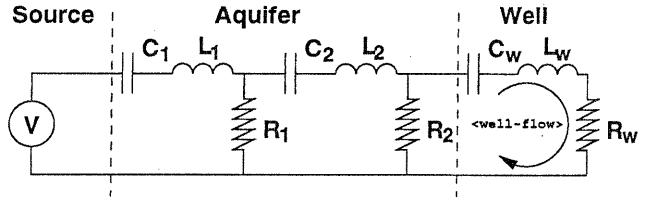


Figure 7: PRET's model of the well/aquifer system. The drive, $V = d_a \sin dt$, simulates a sinusoidal pressure fluctuation in the aquifer; the arrow labeled *<well-flow>* in the network corresponds to the water flow into and out of the well. Note how the *xmission-line* meta-domain and GPN components naturally incorporate the load (the well) into the model.

<force>, or *<water-flow>*. The *xmission-line* meta-domain builds models with an iterative structure, using these *<flow>* and *<effort>* hypotheses as the parallel and series components of the sections and dynamically creating instances of each kind of state variable (e.g. *<flow3>*) as segments are added to the model. Since numeric observations describe specific state variables (e.g. the numerical observation of *<well-flow>* in the *find-model* call), their identifiers are prespecified in the *state-variables* line of the call. Finally, the well/aquifer includes a *nonautonomous* drive term that has an explicit time dependence.

As before, PRET automatically searches the space of possible models, using the *xmission-line* meta-domain template to build models and qualitative and quantitative techniques to test them, until a successful model is found. The result is shown in Figure 7. A perfect model of an infinite-dimensional PDE requires an infinite number of discrete sections, but one can construct approximations using only a few sections, and the fidelity of the match rises with the number of sections². In this case, PRET used two *xmission-line* sections to model the aquifer and one to model the well. This incorporation of the well as an integral part of the model is an important feature of the model-building framework

²Hence the notion of an ODE truncation of a PDE, which is exactly what PRET is constructing here.

described in this paper. Finally, like *linear-plus*, the *xmission-line* meta-domain lets PRET avoid duplication of effort. Connecting arbitrary components in parallel and series creates an exponential number of models, many of which are mathematically equivalent (cf., Thévenin and Norton equivalents, in network theory). This meta-domain avoids this duplication by first limiting the number of possible component combinations in the initial network model (A_1 and B_1 of Figure 5), and then incrementing this structure to a limited depth before attempting another initial network.

Related Work

Much of the pioneering work in the qualitative reasoning (QR) modeling community focuses on reasoning about pre-existing models: simulating them (Kuipers 1986), simplifying and refining them (Weld 1992), or keeping track of which model is appropriate in which regime (Addanki, Cremonini, & Penberthy 1991). QR model construction research has focused on building models from fragments (Bobrow *et al.* 1996; Falkenhainer & Forbus 1991). PRET uses some of the same techniques but has different goals and a different overall approach: it works with noisy, incomplete sensor data from real-world systems and attempts not to "discover" the underlying physics, but rather to find the simplest ODE that accounts for the given observations.

In the QR research that is most closely related to PRET's domains and meta-domains, ODE models are built by evaluating time series using qualitative reasoning techniques and then using parameter estimation to match the resulting model with a given observed system (Capelo, Ironi, & Tentoni 1998). This approach differs from the techniques presented in this paper in that it selects models from a set of pre-enumerated solutions in a very specific domain (linear viscoelastics). Amsterdam's automated model construction tool (Amsterdam 1992) uses a similar underlying component representation (bond graphs) and is applicable to multiple domains. However, it is also somewhat limited; it can only model linear systems of order two or less. The domain/meta-domain framework described in this paper is much more general; it works on linear and non-linear lumped-parameter continuous-time ODEs in a variety of domains, and it uses *dynamic* model generation to handle arbitrary devices and connection topologies.

Conclusion

Model-building domains and meta-domains, coupled with generalized physical networks and a hierarchy of qualitative and quantitative reasoning tools that relate observed physical behavior and model form, provide the flexibility required for gray-box modeling of nonlinear dynamical systems. The two meta-domains introduced in this paper, *linear-plus* and *xmission-line*, use modeling techniques that transcend individual application domains to create rich and yet tractable model search spaces. This framework is flexible as well as powerful; one can use meta-domains directly or customize

them to fit a variety of engineering applications. Both domains and meta-domains adapt smoothly to varying levels of domain knowledge.

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